The notebook for this one is not due until they turn in the Protein Characterization lab next week.

There are 4 GOLD runs to the lab

Human DHFR: 1st Run and 2nd Run

Anthrax bacterial DHFR: 1st Run and 2nd Run

Using only 2 processors per run.

They are NOT making images for every ligand – only a few.

**TROUBLESHOOTING:**

Editing the **configuration** files – make sure they have the EXACT letters and capitalization

**IMPORTANT CONCEPTS:**

The anthrax enzyme is very similar to the human version in 3-d structure

**mtxfor1u72.mol2** vs. **mtx.mol2**

The **mtxfor1u72.mol2** is the ORIGINAL ligand that is used to define the active site. There is a copy of this ligand in the library as a positive control for the docking run (called **mtx.mol2**). But these are technically two different files.

Explain what it means to run the job in the ‘background’.

A ligand database can have thousands of molecules in it that are either very similar – or very different. These ligands came from the **Chembridge Kinase** library that has similar ligands that are supposed to work well against kinase enzymes. (Kinases add phosphates – this is not what DHFR does – but we might find a ligand that binds anyways.)

Most of these compounds will satisfy Lipinski’s rules – because we buy them from a company that is trying to make drugs for humans – and Lipinski’s rules are based off of human drugs.

HELPFUL TIP: When they search for the Lipinski’s data on [www.hit2lead.com](http://www.hit2lead.com) - they can input ALL of the ligand numbers at once (instead of doing it one by one)

**IMPORTANT SKILLS:**

Understanding file structure in Linux operating environment and how to move around in the directories.

Keeping track of all the files we generate.

Creating a list in Excel that is sortable and each of the columns are in separate cells (Bestranking.lst)

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